Augmented Plane-Wave Method for Photonic Band-Gap Materials

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Abstract

We present a numerical method for computing the eigenstates of a photonic band-gap material based on the augmented plane-wave method. The method uses a functional basis set well suited for structures with spherical and cylindrical elements, and allows for fast numerical convergence with a small number of expansion terms. In addition, the method has the ability of dealing with both metallic and dielectric elements without special treatment. The method is applied to an array of long parallel rods with circular cross section.

The first successfully predicted structure to yield a photonic band-gap (PBG) was that of dielectric spheres arranged in a diamond lattice.[1] Since then, there has been considerable effort to elaborate a process for the manufacturing of diamond (or diamond-like) structures at submicron wavelengths. One such approach consists in etching a large number of hole triplets at off-vertical angles in a slab.[2] Another consists in building an orderly stacking of dielectric rods.[3] Yet another consists in etching a series of horizontal grooves into sequentially-grown layers, and etching vertical holes.[4] These structures are variations of the same diamond structure, aligned along either the (1,1,1), (0,0,1), or (1,1,0) directions, respectively. In theoretical treatments, the plane-wave expansion method is commonly used for the computation of band structures and eigenfunctions.[5] However, simple structures such as the ones listed above are amenable to special theoretical treatment. By properly choosing the functional basis set, numerical convergence can be reached with a very small number of expansion terms.

In this letter, we present a theoretical method which uses a functional basis set particularly well suited for structures with spherical and cylindrical elements. Our computational method, based on the augmented plane-wave (APW) method of Slater,[6] uses Bessel functions as a basis set. The method was originally developed for electronic systems, and is usually applied to spherically-symmetric systems with scalar boundary conditions.[7,8] When applied to photonic band-gap materials, the APW method with Bessel functions is most suitable for structures with curved surfaces, and leads to vector boundary conditions.

In addition to yielding fast convergence, the APW method also has the ability of handling different types of materials. Conducting elements had been known to require special theoretical treatment, and several different computational schemes had been used to compute their photonic band structure.[9] However, the APW method can handle metallic elements equally as well as dielectric ones. In this letter, we focus our attention on periodic arrays of long parallel dielectric rods and long conducting rods positioned on a

square lattice. For these structures, the fields can be decomposed into two orthogonal polarizations, and the vector boundary conditions can be reduced to scalar conditions.

The Wigner-Seitz unit cell of the periodic array of rods is shown in Figure 1. In Region I, the basis functions ψ_i (i = 1, 2, . . . n) are given by Bessel functions $J_m(x)$ and $Y_m(x)$, while in Region II, the basis functions are plane waves. Region I is chosen to extend beyond the edges of the cylindrical rod. By adjusting its dimension, we can maximize convergence depending on the geometry of the photonic crystal and the size of the rods. At the interface between Regions I and II, continuity is maintained by matching the Bessel functions to the plane waves using Laurent series:

$$(1) \qquad e^{ik\cdot x} = \sum_{m=-\infty}^{\infty} i^m J_m(|k|x)\, e^{im(\varphi-\varphi_k)}$$

While Eq. (1) garanties continuity of the wavefunction, it does not garanty continuity of its derivative.

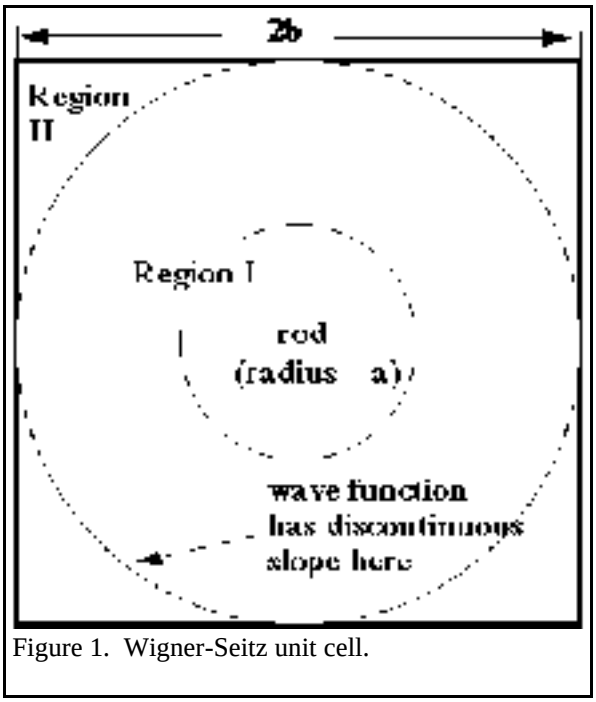

Figure 1. Wigner-Seitz unit cell.

We convert the electromagnetic wave equation with periodic boundary conditions into a variational problem. The problem reduces to solving a non-linear eigenvalue equation of the form det(M) = 0. The matrix elements M^{ij} are given by:

$$(2) \qquad M^{ij} = H^{ij} + S^{ij} - \lambda\Delta^{ij}$$

where

$$(3) \qquad H^{ij} = \int \psi_i^* \, H \, \psi_j \, d\Omega$$

$$(4) \qquad \Delta^{ij} = \int \psi_i^* \, \psi_j \, d\Omega$$

$$(5) \qquad S^{ij} = -\int \psi_i^* \left[\frac{\partial \psi_{j,II}}{\partial r} - \frac{\partial \psi_{j,I}}{\partial r} \right] ds$$

The integration domain Ω in Eqs. (3) and (4) corresponds to the total area of the unit cell defined by Regions I and II. In the first integral, the Hamiltonian operator H is given by $-\nabla^2 + [1 - \varepsilon(r)]$ where $\varepsilon(r)$ is the position-dependent dielectric function. The integral in Eq. (5) is a line integral along the edge of Region I.

By inserting the basis functions into the above equations, we find the following matrix elements

$$(6) \qquad M^{ij} =$$

$$4b^2(k_j^2 - \lambda)\delta_{ij}^2 - 2\pi b^2(k_i\cdot k_j - \lambda)\frac{J_1(\Delta kb)}{\Delta kb} \cdot 2\pi b \sum_m J_m(k_ib)J_m(k_jb)\frac{R'_m(\sqrt{\lambda}b)}{R_m(\sqrt{\lambda}b)} \cos(m\Delta\varphi)$$

where $R_m(x) = b_m J_m(x) + c_m Y_m(x)$ and $R'_m(x)$ is the derivative of $R_m(x)$ with respect to x. The quantities Δk and $\Delta\varphi$ are given by $|k_j - k_i|$ and $|\varphi_j - \varphi_i|$, respectively, and the symbol δ_{ij} represents the Kronecker delta function. In the case of lossless isotropic media, the matrix is real and symmetric.

The coefficients b_m and c_m are chosen to satisfy the boundary conditions within Region I. The boundary conditions depend on the rod material and on the field polarization. In the case where the rods are made of dielectric material, the electric field is continous at the surface for *s* polarization (electric field parallel to the rods) while for *p* polarization (magnetic field parallel to the rods) the magnetic field is continuous. In the case of perfectly conducting rods, the field is zero at the surface for *s* polarization, and the derivative of the field is zero for *p* polarization.

We note that the eigenvalues λ in Eq. (6) appear explicitly in a nonlinear manner. The roots correspond to frequencies of allowed transmission modes through the structure. They are computed using a standard root finding routine for different wavevectors in the periodic lattice. For each $\lambda = (\omega/c)^2$ the determinant of matrix M is found as the product of the diagonal elements in matrix U, which in turn is obtained by LU decomposition of matrix M. Special care must be taken in this procedure to avoid skipping over roots, especially when a pole in the determinant falls near a root.

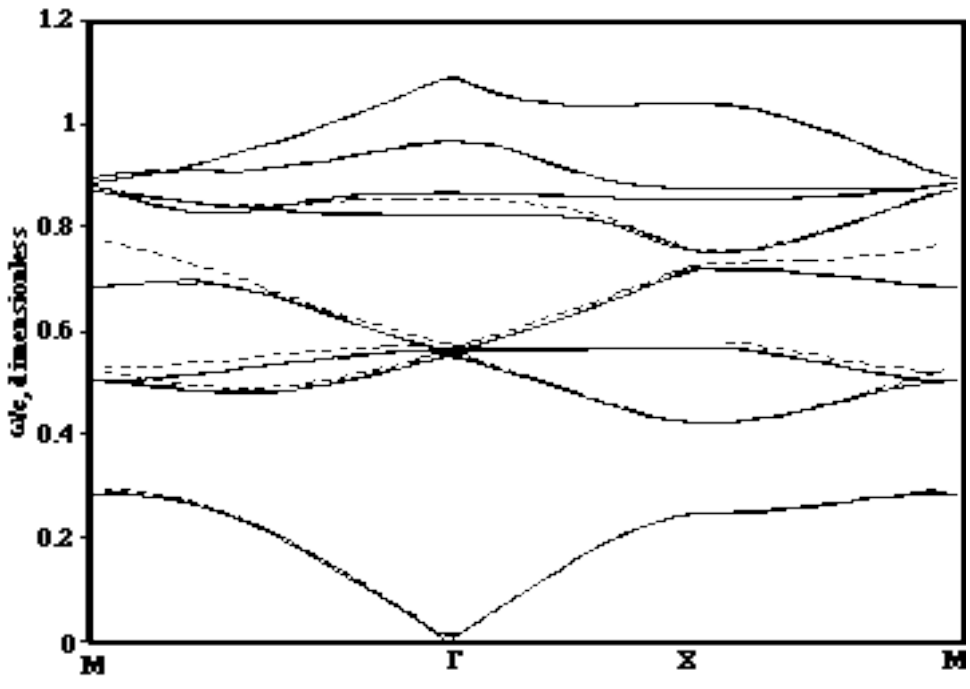

Fig. 2. Band diagram for *s* polarized waves in an array of dielectric rods of index 3.4 computed with a 2x2 (broken line) and 9x9 (heavy line) determinant. Also shown is the band diagram computed from the plane-wave method (light line). The rods have a radius of 0.2 and are located on a square lattice of unit length. The light line is mostly hidden by the heavy line.

We compute the band diagram for two separate cases: (i) dielectric rods and (ii) metallic rods. In the case of dielectric rods, we choose a lattice constant *2b* of 1.0, a rod radius *a* of 0.2, and a dielectric material with an index of refraction of 3.4. Results for *s* polarization are shown in Fig. 2 for a 2x2 and 9x9 determinant. Also shown are results obtained from the plane-wave method developed at MIT.[10] We find excellent agreement between the two methods with as little as 9 APW basis functions.

In the case of perfectly conducting rods, we choose a rod radius of 0.187 and a lattice constant of unity. Results for *s* polarized waves are shown in Fig. 3 for a 2x2, 4x4, and 9x9 determinant. These results are to be compared with those presented in Fig. 6 of Ref. 11 where the Rayleigh scattering method[11] is used

with a 49x49 determinant. Again, excellent agreement can be found with as little as 9 APW basis functions. Although the APW is similar to the Rayleigh scattering method in the case of conductors, the higher rate of convergence of the APW method arises from the continuity conditions imposed at the boundary between Regions I and II.

An area that has been investigated by others for the purpose of determining photonic band structure accuracy is the effective long-wavelength dielectric constant (ε_{eff}) of the heterogeneous medium.[12] In our case we evaluated the first eigenvalue for the pure dielectric case of Figure 2 at $\mathbf{k} = (2\pi)(0.05,0)$. If we were to follow the prescription of Ref. 12 we would plot the computed value of ε_{eff} of versus N and allow N to go to infinity. However, it was found that using only a single basis function, the result was already converged to 5 decimal places. Any such plot would reflect only the noise in the calculational procedure, which is in the 6th decimal place.

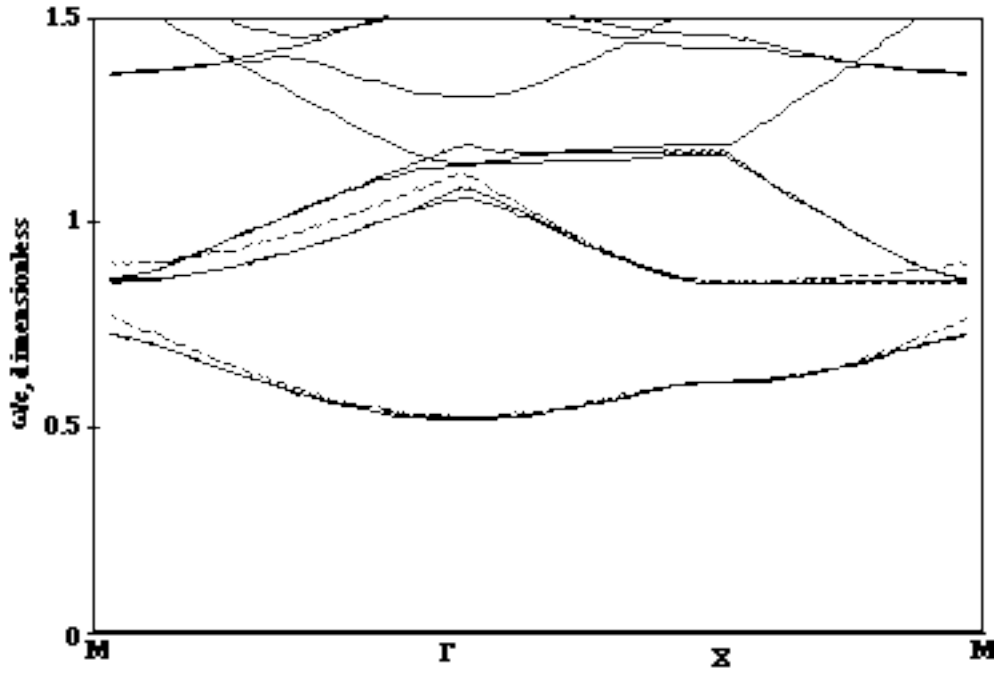

Fig. 3. Band diagram for *s* polarized waves in an array of perfectly conducting rods computed with a 2x2 (broken line), 4x4 (light line), and 9x9 (heavy line) determinant. The rods have a radius of 0.187 and are located on a square lattice of length 1.

Finally, the method described above can also be used to compute the band diagram of three-dimensionally periodic structures. For example, if additional rods are added in orthogonal or non-orthogonal directions, it may be possible to compute the band diagram of structures such as the ones described in Refs. 2 and 3. Furthermore, since the APW method requires a small number of expansion terms to reach convergence, it is well suited for the analysis of structures with very large dimensions, such as supercells containing multiple rods of various types, including defects.

The fast convergence of the APW method is due mostly to the excellent match between the basis set and the geometrical shape of the structure. In general, the APW method should prove to be very useful for a

wide range of structures seeing that, in many cases, photonic band-gap materials have elements with cylindrical or spherical surfaces.

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